

Figure 1

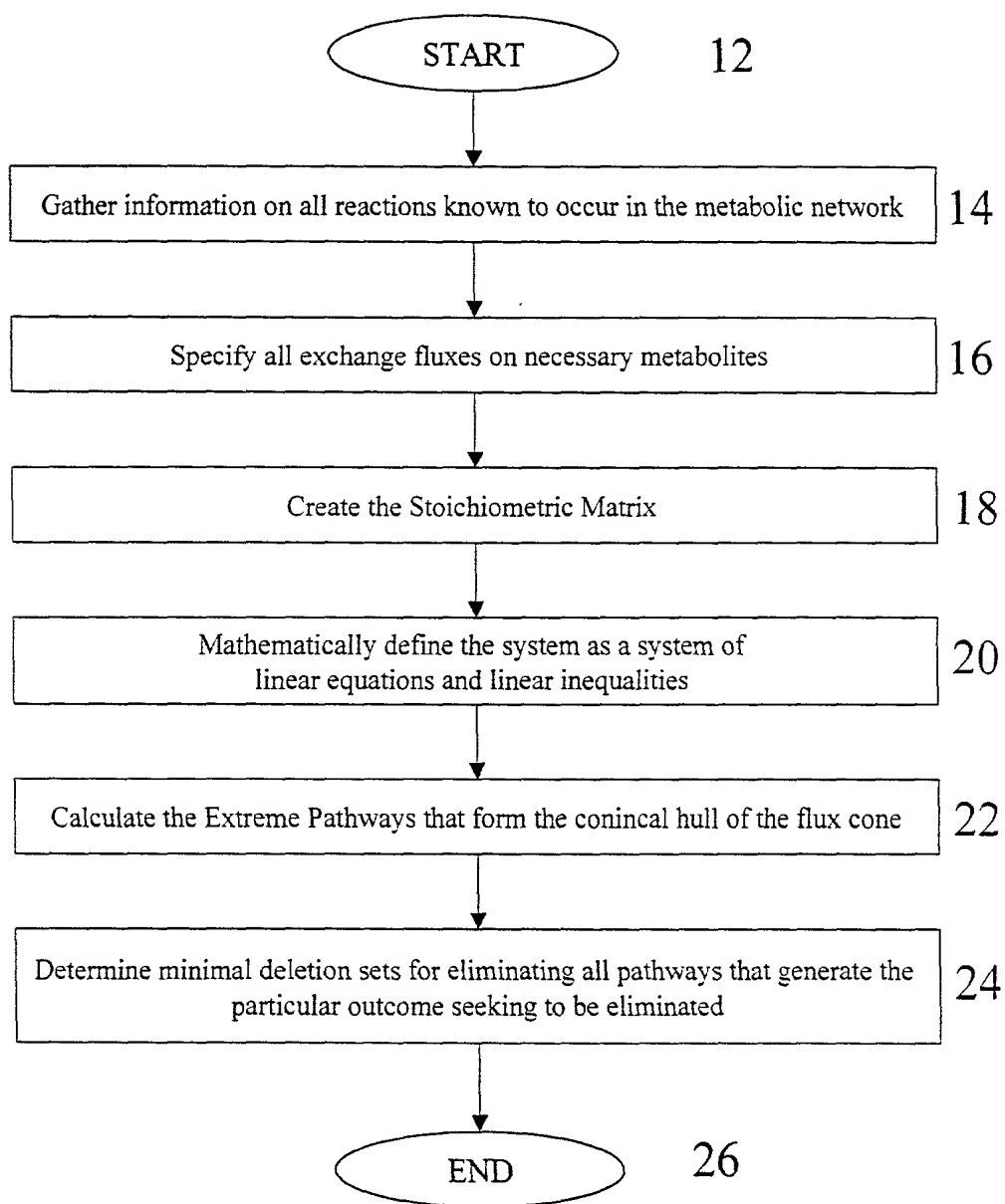


Figure 2

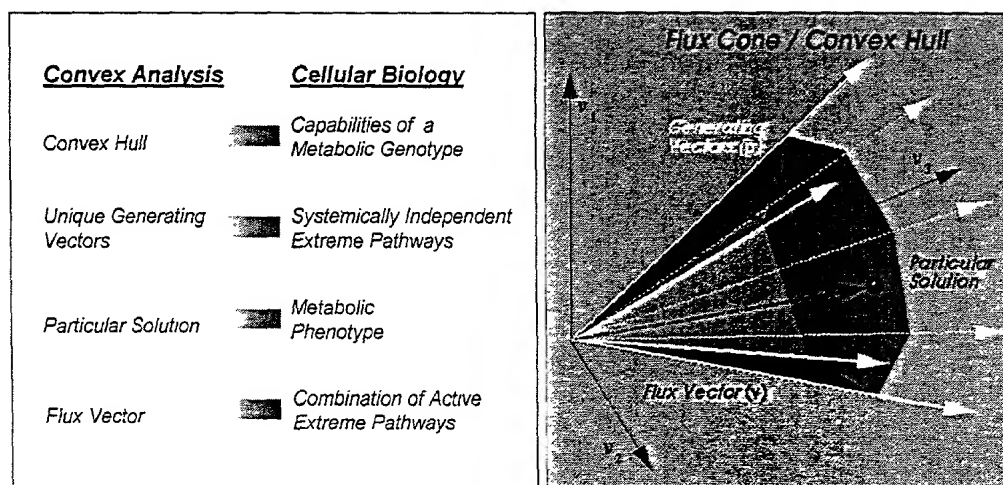
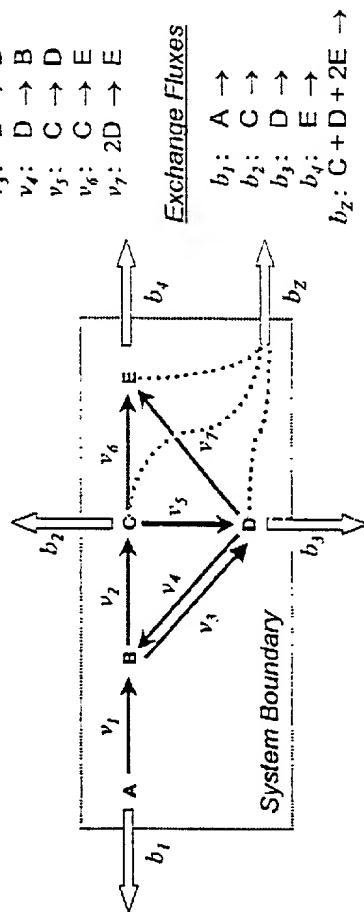


Figure 3

(A) Example Metabolic Reaction Scheme (Linked Outputs)



(B) Mathematical Representation

Steady State Mass Balances

- A: $-v_1 - b_1 = 0$
- B: $v_1 + v_4 - v_2 - v_3 = 0$
- C: $v_2 - v_5 - v_6 - b_2 - b_3 = 0$
- D: $v_3 + v_5 - v_4 - 2v_7 - b_3 - b_4 = 0$
- E: $v_6 + v_7 - b_4 - 2b_5 = 0$

Flux Constraints

- $0 \leq v_1, \dots, v_7 \leq +\infty$
- $-\infty \leq b_1 \leq 0$
- $-\infty \leq b_2 \leq 0$
- $0 \leq b_3 \leq 0$
- $0 \leq b_4 \leq 0$
- $0 \leq b_5 \leq +\infty$

(C) Extreme Pathways

Pathway Number	Internal Fluxes							Exchange Fluxes				
	v_1	v_2	v_3	v_4	v_5	v_6	v_7	b_1	b_2	b_3	b_4	b_5
p'_1	5	0	5	0	0	0	2	-5	-1	0	0	1
p'_2	1	0	1	0	0	2	0	-1	-3	0	0	1
p'_3	0	0	0	0	5	0	2	0	-6	0	0	1
p'_4	0	0	0	0	1	2	0	0	-4	0	0	1
p'_5	6	1	5	0	0	0	2	-6	0	0	0	1
p'_6	4	3	1	0	0	2	0	-4	0	0	0	1
p'_7	6	6	0	0	5	0	2	-6	0	0	0	1
p'_8	4	4	0	0	1	2	0	-4	0	0	0	1
p'_9	0	0	1	1	0	0	0	0	0	0	0	0
p'_{10}	0	1	0	1	1	0	0	0	0	0	0	0

Figure 4

Table 1

Pathway Number	Internal Fluxes								Exchange Fluxes		
	v_1	v_2	v_3	v_4	v_5	v_6	v_7	v_8	b_1	b_2	b_3
1	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	3	0	2	1	0	-4	1
4	0	0	0	0	1	2	0	1	0	-4	1
5	4	1	3	0	0	0	2	1	-4	0	1
6	4	3	1	0	0	2	0	1	-4	0	1
7	4	4	0	0	3	0	2	1	-4	0	1
8	4	4	0	0	1	2	0	1	-4	0	1
9	0	0	1	1	0	0	0	0	0	0	0
10	0	1	0	1	1	0	0	0	0	0	0

Table 1: The set of extreme pathways (p_1, \dots, p_{10}) for the reaction scheme depicted in Figure 2. Pathway 1 and 2 correspond to pathways utilizing both metabolite A and C as substrates, while pathway 3 and 4 utilize only metabolite C. Pathway 5, 6, 7, and 8 utilize metabolite A as the sole substrate. Pathway 9 and 10 show no activity in the exchange fluxes and correspond to internal cycles.

Figure 5

